No-go theorem for topological insulators and high-throughput identification of Chern insulators

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For any symmorphic magnetic space group G, we prove that topological band insulators (with vanishing first Chern numbers) cannot have a ground state composed of a *single*, energetically isolated band. This no-go statement means that such topological insulators cannot be realized in tight-binding models with a single, filled, low-energy band. An implication is that the minimal dimension of the tight-binding Hamiltonian (at each wave vector) is *four*, if the topological insulator is stable, i.e., the filled bands remain topological upon addition of nontopological bands. Otherwise, if the topological insulator is unstable, the minimal dimension is *three*. In addition to our no-go statement, we present a surefire recipe to model Chern insulators and unstable topological insulators, by energetically splitting elementary band representations; this recipe, combined with recently constructed Bilbao tables on band representations, can be systematized for high-throughput identification of magnetic and time-reversal-invariant topological materials. All stated results follow from our theorem which applies to any single, isolated energy band of a G-symmetric Schrödinger-type or tight-binding Hamiltonian: for such bands, being topologically trivial (in the category of complex vector bundles) is equivalent to being a band representation of G.

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I. INTRODUCTION

A real-space representation of topological band insulators is emerging from various directions [1–7], with the unifying theme that topological nontriviality is fundamentally linked to an obstruction to constructing Wannier functions [4,8–11]. In band insulators, the existence of Wannier functions has traditionally justified that electrons form exponentially localized wave packets in real space, and therefore the effects of local disturbances are short ranged [12–14]. Despite the similarity of such localized wave packets with the electronic orbitals of atoms, there remains a sharp, group-theoretic distinction between solids and a lattice of spatially isolated atoms: Wannier functions and atomic orbitals may transform differently under crystallographic point-group symmetries that preserve at least one spatial point, as exemplified by rotations or time reversal. This distinction was first pointed out by Soluyanov and Vanderbilt [2] for the Kane-Mele [15–20] topological insulator in Wigner-Dyson symmetry class AII [21]: in this phase it is impossible to construct a Kramers pair of Wannier functions centered at the same spatial point [2,4,5], as comparatively illustrated in Figs. 1(c) and 1(d). Alternatively stated, the Wannier functions in the Kane-Mele phase cannot locally represent time-reversal symmetry.

In the Kane-Mele model, the bands which are filled at zero temperature exemplify a localizable topological band. By *"localizable"* we mean that the band is spanned by exponentially localized Wannier functions; by *"localizable topological band"* we mean a localizable band whose Wannier functions are obstructed from satisfying the following *local symmetry condition*: for any spatial point ϖ, all Wannier functions centered at ϖ form a representation of all point-group symmetries that preserve ϖ. If a localizable topological band is the filled band of an insulator, we refer to this insulator as a localizable topological insulator.[1] Included in this category are all ($d \leqslant 3$)-dimensional topological insulators with vanishing first Chern class ($c_1 = 0$), and whose protective symmetries are classified by the magnetic space groups [22] (numbering 1651 in $d = 3$). Both time-reversal-invariant [5,23] and magnetically ordered [24] insulators are considered; in the former case, the first Chern class vanishes by symmetry [25]. Examples of localizable topological insulators that have materialized in laboratories include Bi_2Se_3 [26,27] [a three-dimensional (3D) $\mathbb{Z}_2$ topological insulator] [28–31], SnTe [32–34], and KHgSb [35–37] (topological crystalline insulators) [38–48]. In contrast to these laboratory examples, not all localizable topological insulators have robust boundary states: they may instead manifest nontrivial windings in the holonomy of Bloch functions over Brillouin-zone loops [41,49,50].

This work presents rigorous results that apply in any spatial dimension d and to solids whose magnetic space groups (denoted G) are symmorphic, i.e., G consists only of symmetries that are factorizable into products of point-group symmetries with lattice translations. A case in point is SnTe, whose rocksalt structure has the symmetry of the symmorphic space group 225; in contrast, nonsymmorphic KHgSb is symmetric under glide, which is the product of a reflection with half a lattice translation.

[1]Our results do not immediately apply to band topological superconductors, which have an additional particle-hole and/or chiral symmetries in the Bogoliubov–de Gennes formalism [82]. The possibility to formulate band representations for superconductors remains an open and interesting question.

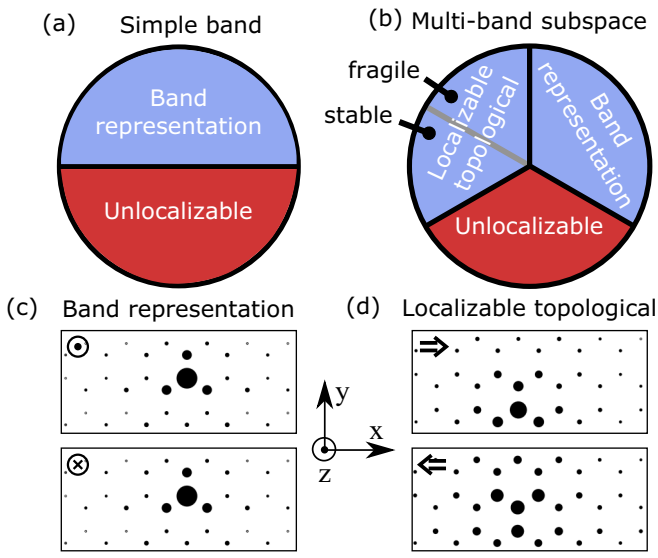

FIG. 1. (a), (b) Topological categorization of a simple band [(a)] and ($N > 1$)-band subspaces [(b)]. In spatial dimension $d \leqslant 3$, being localizable is equivalent to having vanishing first Chern class (c_1), as colored blue; phases with $c_1 \neq 0$ are colored red. (c), (d) Comparison of Wannier functions in a nontopological and topological (Kane-Mele) phase, with the symmetry of a honeycomb lattice with staggered sublattices. The size of each dot measures the weight of the Wannier function on a lattice site; the expectation value of spin for each Wannier function is indicated by an arrow in the inset. (c) In the nontopological phase, Wannier functions form Kramers pairs centered on the same lattice site. (d) In the topological Kane-Mele phase, every Wannier function is centered on a different lattice site.

Our first result is a no-go statement: a localizable topological band cannot be a simple band. By "simple" we mean a single band that is nondegenerate (in energy) throughout the Brillouin torus. A localizable band spanned by *locally symmetric* Wannier functions is defined to be a band representation [51–54]. Colloquially, a band representation resembles a lattice of locally symmetric atomic orbitals [7] [as illustrated in Fig. 1(c)], and is sometimes referred to as an atomic insulator [55,56]. The contrapositive of the no-go statement is that any simple band that is not a band representation cannot be localizable, i.e., it has nontrivial first Chern class ($c_1 \neq 0$); this is presented pictorially in Figs. 1(a) and 1(b), which compares the topological categorization of simple bands with nonsimple bands. To clarify, each of Figs. 1(a) and 1(b) is a categorization of G-symmetric bands with the same, fixed number of linearly independent Bloch functions at each wave vector.[2] Equivalently, we mean a categorization of fixed-rank, G-equivariant vector bundles [57,58], which differs from stably equivalent classifications based on K-theory [46,59,60] or symmetry-based indicators [56].

Our results follow from a theorem that applies to simple bands occurring as energy eigenfunctions of Schrödinger-type or tight-binding Hamiltonians with the symmetry G: for such simple bands, being topologically trivial (in the category of complex vector bundles) is equivalent to being a band representation of G.

We have adopted a definition of topological triviality that is standard in the theory of complex vector bundles [61,62], but is not universally adopted in the literature of topological band insulators. In particular, we caution that a recent work [5] defines triviality as being a band representation, but this is *not* equivalent to triviality in the theory of complex vector bundles. The bundle-theoretic notion of topological triviality, as well as its relation to the existence of Wannier functions, is reviewed in Sec. II A. In Sec. II B, we describe how the inclusion of crystallographic point-group symmetry leads to two distinct categories for topologically trivial bands, which we illustrate with well-known examples. A more general and precise statement of the theorem is provided in Sec. III. One may question if there is a loss of generality in our restriction to symmorphic G. Actually, the hypothesis of the theorem becomes superfluous for all nonsymmorphic magnetic space groups with at least one nonsymmorphic element (a symmetry that is partially a translation by a fraction of a lattice vector, e.g., screw or glide), and possibly even for the minority of nonsymmorphic groups without nonsymmorphic elements; these groups just do not allow for simple bands.[3]

Applications of our theorem include (i) the establishment of a minimal rank for the tight-binding Hamiltonian of any localizable topological insulator with symmorphic symmetry. By "rank" we mean the dimension (at each wave vector) of the Hamiltonian, or equivalently the number of orthogonal Wannier functions that span the tight-binding Hilbert space in one primitive unit cell. The ground state of a tight-binding Hamiltonian refers to its low-energy, filled bands. The minimal rank depends on whether the localizable topological ground state is stable, i.e., whether it remains localizable topological upon addition of band representations; stable phases are classified by topological K-theory [46,59,60], and unstable (or "fragile" [55][4]) phases manifest in a finer classification of vector bundles [57,58]. We find that the minimal rank is four in the stable case, and three in the fragile case. A second application of our theorem is (ii) a surefire recipe to design and/or identify bands with nontrivial Chern number, as well as fragile localizable topological bands; this recipe may be systematized for high-throughput identification of magnetic and time-reversal-invariant topological materials. Points (i) and (ii) and other applications are elaborated in Sec. VIII.

[2]We do not require that a rank-($N > 1$) band is connected by band touchings.

[3]For space groups with at least one nonsymmorphic element, bands must be nontrivially connected as a graph due to the monodromy of symmetry representations, as proven in the Supplemental Material of [7]. Less general proofs exist for solids without spin-orbit coupling in [92] and for band representations only in [76]. All type I (without time-reversal symmetry) and II (with time-reversal symmetry by itself) nonsymmorphic magnetic space groups have nonsymmorphic elements in $d = 2$, but not in $d \geqslant 3$. For nonsymmorphic space groups without nonsymmorphic elements, we are not aware of a general proof that simple bands do not exist; however, this seems empirically to be true for specific case studies in $d = 3$ [24,76,92,93].

[4]"Fragile" is a symmetry-enriched analog of "nontrivial but stably trivial" in bundle theory [4,62].

Section VII generalizes the theorem to half-integer-spin representations of point-group symmetries, with application to solids with spin-orbit coupling. After establishing a few preliminary results on space groups and their representations in Sec. IV, we prove in Sec. V that a simple band that is a band representation is topologically trivial. The converse statement, that topologically trivial simple bands are band representations, is proven in Sec. VI. Finally, in Sec. IX, we summarize our results from the perspective of establishing rank constraints for bands.

For quick reference, we collect [in (i)–(iv) below] the definitions of several key terms used throughout this work. Many of these definitions are stated more elaborately in Secs. I and III. A version of our theorem that is most physically applicable is stated in (v) below; a more general statement of the theorem can be found in Sec. III.

(i) An *N-band subspace* comprises N orthogonal Bloch functions at each wave vector ($\boldsymbol{k}$) in the Brillouin d-torus T^d. An N-band subspace that occurs as an energy eigenfunction of a Hamiltonian is assumed to be energetically isolated, i.e., at each wave vector, an energy gap separates this subspace from all other higher- and lower-energy bands. Often, we will use *band* as a shorthand for an N-band subspace; N should be deducible from the context. A one-band subspace is a *simple band*, and a multiband ($N > 1$) subspace is a nonsimple band.

(ii) A *localizable* N-band subspace (in short, localizable band) is spanned by orthogonal Wannier functions (numbering N in each primitive unit cell); all Wannier functions referred to in this work should be understood as exponentially localized. For a localizable band that has the symmetry of a magnetic space group G (in short, is G symmetric), the corresponding Wannier functions must form a representation of G.

(iii) A rank-N *band representation* of G is a localizable, G-symmetric, N-band subspace that is *locally symmetric*. The local symmetry condition is as follows: For any spatial point $\boldsymbol{\varpi}$, all Wannier functions centered at $\boldsymbol{\varpi}$ form a finite-dimensional representation of the subgroup of G that preserves $\boldsymbol{\varpi}$. If a localizable band is obstructed from being locally symmetric, it is defined to be a *localizable topological* band. If a localizable topological band is the filled band of an insulator, we refer to this insulator as a localizable topological insulator.

(iv) An N-band subspace is *topologically trivial* in the category of complex vector bundles, if there exist Bloch functions which span the N-dimensional vector space at each wave vector, and are continuous and periodic over the Brillouin torus T^d. Being topologically trivial is equivalent [25] to being localizable. For $d<4$, being topologically trivial is equivalent [58,63] to a vanishing first Chern class, i.e., the first Chern number vanishes in any closed two-dimensional submanifold of T^d.

(v) *Theorem.* Suppose a simple band is an energy eigenfunction of a Schrödinger-type or tight-binding Hamiltonian, which has the symmetry of a symmorphic magnetic space group G. Some physically reasonable conditions (elaborated in Sec. III) are assumed to ensure that the Hamiltonian is self-adjoint, analytic in $\boldsymbol{k}$, and has a point spectrum. Our theorem states that for such a simple band, being topologically trivial (in the category of complex vector bundles) is equivalent to being a band representation of G.

II. EXISTENCE OF WANNIER FUNCTIONS FOR TOPOLOGICALLY TRIVIAL BANDS

Our theorem may be viewed as a symmetry-refined analog of known relations between topological nontriviality and an obstruction to the existence of Wannier functions; these relations will be briefly reviewed in Sec. I A, and subsequently in Sec. II B we will introduce crystallographic point-group symmetry to further motivate our theorem.

A. Insulators with discrete translational symmetry

Let us first consider d-dimensional band insulators in Wigner-Dyson symmetry class A, with the additional symmetry of discrete translations in d-independent directions. A well-recognized form of topological nontriviality arises for two-dimensional insulators whose Hall conductance $C_1 e^2/h$ is quantized in units of fundamental constants; C_1 is the first Chern number (also known as the Thouless-Kohmoto-Nightingale–den Nijs [64] invariant) of the filled bands. Generally, for d-dimensional solids, a nonzero C_1 in any two-dimensional closed submanifold of the Brillouin d-torus (T^d) is equivalent to a nonzero first Chern class ($c_1 \neq 0$) [25]. The foundational works of Nenciu [14], Panati [25], and Brouder *et al.* [10] have culminated in an equivalence between the vanishing of the first Chern class ($c_1 = 0$) and the existence of Wannier functions (i.e., localizability) in ($d \leqslant 3$)-dimensional solids. This equivalence broadly applies to N-band subspaces for any $N \geqslant 1$, including the case of simple bands ($N = 1$); we shall refer to N as the rank.

For $d \leqslant 3$, the vanishing of the first Chern class ($c_1 = 0$) is equivalent to the band subspace being topologically trivial [58,63]. Throughout this paper, we adopt the standard definition of topological triviality from the theory of vector bundles [61]. Applied to the Bloch problem, an N-band subspace is topologically trivial if there exist Bloch functions[5] which span the N-dimensional vector space at each quasimomentum ($\boldsymbol{k}$), and are continuous and periodic over the Brillouin d-torus T^d. To translate between band- and bundle-theoretic languages, the N Bloch functions form an N-dimensional vector space at each $\boldsymbol{k} \in T^d$; the union of all such vector spaces over the base space T^d defines a rank-N complex vector bundle. If there exist N (continuous and periodic) sections that span the N-dimensional vector space at each $\boldsymbol{k}$, we say that this bundle is topologically trivial in the category of complex vector bundles. We will interchangeably use "sections" with "Bloch functions," and "vector bundles" with "bands." For most of this work, "topological triviality" should implicitly be understood as for complex vector bundles, though we shall remark briefly on real vector bundles in Sec. VIII C.

The above definition of triviality applies to any spatial dimension d. Especially for $d \geqslant 4$, which is physically realizable in cold atoms [65,66] and electrical circuits [67–69],

[5]Bloch functions do not have to correspond to energy bands; sometimes these are referred as quasi-Bloch functions [10,25,72].

being topologically trivial more stringently constrains the band subspace than having a trivial first Chern class: additional constraints include (but is not exhausted by) [57,62] the triviality of all higher Chern classes. However, a nontrivial higher Chern class can only be realized by multiband subspaces; in the absence of crystallographic symmetry, simple bands are fully classified by the first Chern class in any dimension d [62].

B. Two categories of topologically trivial bands with the inclusion of point-group symmetry

The inclusion of point-group symmetry allows us to distinguish between two categories of topologically trivial bands: band representations and localizable topological bands. As stated in the Introduction, a band representation is a topologically trivial band that satisfies the local symmetry condition. Here, we offer an equivalent,[6] and more constructive, definition: any band representation of a magnetic space group G is attained by specifying a spatial point $\boldsymbol{\varpi}$, and specifying a finite-numbered set of Wannier functions that transform in a representation of the subgroup (denoted $G_{\boldsymbol{\varpi}}$) of G that preserves $\boldsymbol{\varpi}$. By applying all elements of G on said Wannier functions, we obtain an infinite-dimensional representation of G that is a band representation (BR). Precisely, a BR of G with position $\boldsymbol{\varpi}$ is an induced representation of $G_{\boldsymbol{\varpi}} \subset G$. For illustration, let us consider a BR of type-II magnetic space group $P3m1$, which is the symmetry of a honeycomb lattice with staggered sublattices. We pick $\boldsymbol{\varpi}$ to be a honeycomb vertex, whose associated subgroup $G_{\boldsymbol{\varpi}}$ is generated by a threefold rotation, spatial reflection, and time reversal. We specify a Kramers pair of Wannier functions that transform in an irreducible, spinor representation of $G_{\boldsymbol{\varpi}}$ [as illustrated in Fig. 1(c)], then apply all elements of G on said Wannier functions to obtain a BR. Beyond this model, Wannier functions of BRs are commonly applied as exponentially localized, locally symmetric basis functions for a G-symmetric tight-binding model [4,7].

Wannier representations of G which are not BRs are referred to as localizable topological. To illustrate a localizable topological band, let us elaborate on the low-energy filled band of the Kane-Mele $\mathbb{Z}_2$ topological insulator with the same symmetry as the staggered honeycomb lattice; we further assume time-reversal symmetry, which guarantees that the filled bands have vanishing first Chern class $c_1 = 0$ [25]. By applying all elements of G to the two representative Wannier functions illustrated in Fig 1(d), we attain a nonsimple band that is localizable, i.e., topologically trivial in the category of complex vector bundles. Yet, the two generating Wannier functions are centered on distinct honeycomb sublattices, and hence do not form a spinor representation of time reversal; after all, time reversal, being a spatially local operation, always relates two orthogonal Wannier functions centered at the same point.

A second example of a localizable topological band is the filled band of a reflection-symmetric insulator with a nonzero mirror Chern number [70] (this number will be explained below). This is exemplified by the SnTe class of topological crystalline insulators [32], but for conceptual simplicity we consider a simpler model, on a two-dimensional lattice with an out-of-plane reflection axis. Any point on the plane is then invariant under a reflection symmetry that squares to identity (modulo a phase), i.e., the reflection symmetry is an element of $G_{\boldsymbol{\varpi}}$ for any $\boldsymbol{\varpi}$. Suppose the filled band is the sum of two simple bands, each transforming in opposite representations of the reflection symmetry; each simple band further carries a nonzero first Chern number known as the mirror Chern number, but the sum of the mirror Chern numbers (in odd and even representations) vanishes. The latter implies that the filled band is topologically trivial in the category of complex vector bundles, hence, one may certainly construct Wannier functions which span the filled band. Yet, the nonzero mirror Chern number implies it is impossible to construct two representative Wannier functions which generate all other Wannier functions (by application of all space-group elements), and which also transform in a representation of reflection symmetry.[7]

Before the discovery of $\mathbb{Z}_2$ topological insulators [15,16,70], and topological crystalline insulators [32,35], it was widely believed that a topologically trivial N-band subspace with G symmetry is necessarily a BR of G. The two illustrations above provide counterexamples where $N = 2$. Our contribution is to prove that this belief holds for $N = 1$, and for any symmorphic magnetic space group G in any spatial dimension d. By "symmorphic" we mean G is a semidirect product of its translational subgroup $T \subset G$ with the quotient group G/T, as further elaborated in Sec. IV A. This $N = 1$ result may be viewed as a symmetry-refined analog of the no-go statement mentioned in Sec. II A: not only are simple bands unable to realize nontrivial higher Chern classes, we find that they also cannot realize localizable topological insulators in symmorphic magnetic space groups.

III. STATEMENT OF THEOREM

Our main result is encapsulated in the following theorem, which applies for any spatial dimension d.

Theorem 1. For any simple band whose corresponding projection operator is analytic throughout T^d, being a band representation of a symmorphic magnetic space group G is equivalent to being topologically trivial in the category of complex, unit-rank vector bundles. The latter condition is known to be equivalent [62] to a vanishing first Chern class.

[6] This equivalence is proven in Appendix A.

[7] Let us prove this by contradiction. Assume that the representative pair of Wannier functions (w_1 and w_2) forms a representation of reflection. If w_1 and w_2 are centered on distinct spatial positions, then each of the two must form a single-dimensional representation of reflection (but with opposite mirror eigenvalues). This would imply that a Wannier representation exists for the band subspace in the even representation of reflection, which contradicts the nonzero first Chern number in that subspace. If w_1 and w_2 are centered at the same point, it is possible that they form a two-dimensional representation of reflection; however, such a representation is always reducible to two one-dimensional representations, hence, we arrive at the same contradiction.

Let us discuss the physical scenarios where the above-stated assumptions on the simple band are attained. The simple band may be an energy eigenfunction of a G-symmetric Schrödinger Hamiltonian $H_0 = -\bigtriangleup + V(\boldsymbol{r})$ with energy eigenvalue $\varepsilon_{\boldsymbol{k}}$ that is nondegenerate at all $\boldsymbol{k}$; this nondegeneracy shall be referred to as a gap condition. To ensure that $e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} H_0 e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$, at each $\boldsymbol{k}$, is self-adjoint, analytic,[8] and has a point spectrum, $V(\boldsymbol{r})$ has to satisfy certain physically reasonable conditions,[9] e.g., for $d \leqslant 3$ it is sufficient that V is square integrable over the primitive unit cell. Alternatively, H_0 might be a tight-binding Hamiltonian whose matrix elements decay exponentially in real space, which ensures that the Fourier transform of H_0 is analytic throughout T^d [13]. The analyticity and gap conditions ensure that the projection operator to the simple band is analytic at all $\boldsymbol{k}$ [4,25,71,72].

IV. PRELIMINARIES

A. Space groups

For any magnetic space group G that is symmorphic, there exists a point where each $g \in G$ is the composition [denoted $(p|\boldsymbol{R})$] of a transformation p that preserves said point, and a translation by a Bravais-lattice vector $\boldsymbol{R}$; generally, $p = p(g)$ and $\boldsymbol{R} = \boldsymbol{R}(g)$, but we shall omit the arguments. We employ BL as a shorthand for the Bravais lattice (e.g., $\boldsymbol{R} \in BL$) and RL for the dual (reciprocal) lattice to BL.

The set of p defines the point group $\mathcal{P}$ of G, which is isomorphic to G/T [73]. p is specified by (i) a $d \times d$ real orthogonal matrix $\check{p}$ that acts on real space, as well as (ii) a $\mathbb{Z}_2$ index $s_p = \pm 1$ which indicates whether or not p involves a time-reversal operation; $g = (p|\boldsymbol{R})$ then acts on $(d+1)$-dimensional space-time as $\boldsymbol{r} \to g \circ \boldsymbol{r} := \check{p}\boldsymbol{r} + \boldsymbol{R}$ and $t \to s_p t$. In magnetic space groups without time-reversal symmetry, $s_p = 1$ for all $p \in \mathcal{P}$. The standard multiplication rule for magnetic space groups is

$$(q|\boldsymbol{R}')(p|\boldsymbol{R}) = (qp|\check{q}\boldsymbol{R} + \boldsymbol{R}') \text{ with } s_{qp} = s_q s_p, \qquad (1)$$

where the presence of $\check{q}$ reflects the noncommutativity of translations and point-group operations.

A notion that is useful to characterize Wannier functions is a Wyckoff position $\boldsymbol{\varpi}$ of G; $\boldsymbol{\varpi}$ is defined as a spatial coordinate in $\mathbb{R}^d$ with an associated symmetry group $G_{\boldsymbol{\varpi}} \subset G$. $G_{\boldsymbol{\varpi}}$, the site stabilizer, comprises all elements of G that preserve $\boldsymbol{\varpi}$, i.e., for any $g \in G_{\boldsymbol{\varpi}}$, $g \circ \boldsymbol{\varpi} = \boldsymbol{\varpi}$. If $g \circ \boldsymbol{\varpi} - \boldsymbol{\varpi}$ is a BL vector for all $g \in G$ (equivalently, $G/G_{\boldsymbol{\varpi}} \cong T$), then we say that $\boldsymbol{\varpi}$ has unit multiplicity.

B. General representations of space groups

A simple band is spanned at each $\boldsymbol{k}$ by a Bloch function $\psi_{\boldsymbol{k}}$, whose phase is not uniquely defined. The projection $P(\boldsymbol{k}) = |\psi_{\boldsymbol{k}}\rangle\langle\psi_{\boldsymbol{k}}|$ is periodic over T^d. By the assumptions stated in the theorem, $P(\boldsymbol{k})$ is analytic at all $\boldsymbol{k} \in T^d$, and $\psi_{\boldsymbol{k}}$ forms a general representation of G. By this, we mean there exists a map from $g \in G$ to a unitary $\rho_g(\boldsymbol{k}) \in U(1)$, such that

$$\hat{g}\,\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \rho_g(\boldsymbol{k})\psi_{s_p\check{p}\boldsymbol{k}}(\boldsymbol{r}). \qquad (2)$$

Here, $\hat{g}$ is defined as a representation of G that acts on functions of real space as $\hat{g}f(\boldsymbol{r}) = \overline{f(g^{-1}\circ\boldsymbol{r})}^{s_p}$, where $\bar{a}^1 := a$ and $\bar{a}^{-1} := \bar{a}$ (the complex conjugate).[10]

While Eq. (2) and the remaining proof is specific to Schrödinger wave functions, the proof is essentially unchanged if we replace $\psi_{\boldsymbol{k}}(\boldsymbol{r})$ by a finite-dimensional vector in a tight-binding basis of Löwdin-orthogonalized orbitals [74].

From the action of $\hat{g}$ on $\psi_{\boldsymbol{k}}(\boldsymbol{r})$, we deduce that ρ_g may be factorized into translational and point-group components as

$$\rho_{(p|\boldsymbol{R})}(\boldsymbol{k}) = \overline{\rho_{(E|\boldsymbol{R})}(\check{p}\boldsymbol{k})}^{s_p}\rho_{(p|\boldsymbol{0})}(\boldsymbol{k}) = e^{-is_p\check{p}\boldsymbol{k}\cdot\boldsymbol{R}}\rho_{(p|\boldsymbol{0})}(\boldsymbol{k}), \qquad (3)$$

where E denotes the identity element of the point group, and $\rho_{(E|\boldsymbol{R})}(\boldsymbol{k}) = \mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{R}}$ describes the translational property of Bloch functions. That such a factorization exists reflects that G is a semidirect product of its translational and point subgroups. A useful implication of Eq. (3) is that $\rho_{(p|\boldsymbol{R})}(\boldsymbol{0}) = \rho_{(p|\boldsymbol{0})}(\boldsymbol{0})$ is independent of $\boldsymbol{R}$. Owing to

$$\hat{h}(\hat{g}\,f(\boldsymbol{r})) = \overline{f(\,g^{-1}\circ(h^{-1}\circ\boldsymbol{r})\,)}^{s_q s_p} = \overline{f((hg)^{-1}\circ\boldsymbol{r})}^{s_{qp}} \qquad (4)$$

for all $g = (p|\boldsymbol{R})$, $h = (q|\boldsymbol{S}) \in G$ and hg defined through Eq. (1), the representation $\hat{g}$ is linear (i.e., $\hat{h}\hat{g} = \widehat{hg}$), and therefore

$$\rho_{(q|\boldsymbol{S})}(s_p\check{p}\boldsymbol{k})\,\overline{\rho_{(p|\boldsymbol{R})}(\boldsymbol{k})}^{s_q} = \rho_{(q|\boldsymbol{S})(p|\boldsymbol{R})}(\boldsymbol{k}). \qquad (5)$$

Under a phase redefinition (or change in gauge) of $\psi_{\boldsymbol{k}}$, $\psi_{\boldsymbol{k}}$ and $\rho_g(\boldsymbol{k})$ transform as

$$\psi_{\boldsymbol{k}} \to e^{i\phi(\boldsymbol{k})}\psi_{\boldsymbol{k}}, \quad \rho_g(\boldsymbol{k}) \to e^{-i\phi(s_p\check{p}\boldsymbol{k})}\rho_g(\boldsymbol{k})e^{is_p\phi(\boldsymbol{k})}. \qquad (6)$$

Under such a gauge transformation, $\psi_{\boldsymbol{k}}$ can be made analytic at $\boldsymbol{k}$, for every $\boldsymbol{k} \in T^d$; the existence of such analytic local sections is guaranteed by the assumed analyticity of the projection $P(\boldsymbol{k})$.[11] Whether $\psi_{\boldsymbol{k}}$ can be made analytic throughout and periodic over T^d depends not just on the analyticity of $P(\boldsymbol{k})$, but also requires that there are no topological obstructions in the category of complex vector bundles [25,72]. That is, if the simple band is topologically trivial, $\psi_{\boldsymbol{k}}$ exists that is continuous and periodic over T^d; the continuity condition on $\psi_{\boldsymbol{k}}$ can be further strengthened to analyticity throughout T^d.[12]

[8] Precisely, $e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} H_0 e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ should be in the entire analytic family of type A, as defined in [71].

[9] Dimension-dependent conditions on V are stated in [71], Theorem XIII.99: $V \in L^p(\text{unit cell}, d^d\boldsymbol{r})$ for $p = 2$ if $d \leqslant 3$, $p > 2$ if $d = 4$ and $p = d/2$ if $d \geqslant 5$.

[10] This action of g on f defines a regular representation [84] which is known to be linear.

[11] This follows from analytic perturbation theory, e.g., see [108] for the tight binding H_0, and the Kato-Rellich theorem in [71] for the Schrödinger H_0.

[12] A complex neighborhood of T^d may be identified as a domain of holomorphy in $\mathbb{C}^d$ and therefore a Stein space. Solving the second Cousin problem over a Stein space is equivalent to proving the existence of a global analytic section for a topologically trivial line bundle; this has been carried out in [109]. See also related discussions falling under the "Grauert-Oka principle" [101,110] in [25,111]. In fact, the non-Abelian second Cousin problem has also been solved using sheaf theory [101–103]; this implies, for a topologically trivial band of rank $N \geqslant 1$, that there exist analytic and periodic Bloch functions which span the N-dimensional vector space at each $\boldsymbol{k}$.

C. Localizable representations of space groups

Henceforth it should be understood that any function of $\boldsymbol{k}$ that is described as "periodic" (respectively "analytic") is periodic over T^d (respectively analytic throughout T^d). Being both analytic and periodic are necessary and sufficient [13] conditions for the Fourier transform of $\psi_{\boldsymbol{k}}$,

$$w_{\boldsymbol{R}}(\boldsymbol{r}) = \frac{1}{\sqrt{|T^d|}} \int_{T^d} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} \psi_{\boldsymbol{k}}(\boldsymbol{r}) d\boldsymbol{k} \tag{7}$$

to be exponentially localized; $|T^d|$ above denotes the volume of T^d. Such a localized wave packet is referred to as a Wannier function; any band subspace which forms a general representation of G and is spanned by Wannier functions is said to be a localizable representation of G.

D. Band representations of space groups

As motivated in the Introduction, not all localizable representations of G are BRs of G [75]. For the purpose of proving our theorem, we may specialize the definition of BRs to simple bands with symmorphic G symmetry: a localizable representation of G given by $\{w_{\boldsymbol{R}}\}_{\boldsymbol{R}\in BL}$ [cf. Eq. (7)] is a BR of G with unit-multiplicity Wyckoff position $\boldsymbol{\varpi}$, if $w_{\boldsymbol{R}}$ forms a representation of the site stabilizer $G_{\boldsymbol{\varpi}+\boldsymbol{R}} \cong \mathcal{P}$, for any $\boldsymbol{R} \in BL$. This may be viewed as a precise restatement of the local symmetry condition first formulated in the Introduction. The general definition of BRs that is applicable to nonsimple bands and nonsymmorphic space groups is provided in Appendix A.

It is instructive to physically interpret [76] $\boldsymbol{\varpi}$ as the Wannier center:

$$\bar{\boldsymbol{r}} := \langle w_{\boldsymbol{0}}|\boldsymbol{r}|w_{\boldsymbol{0}}\rangle = \frac{1}{|T^d|}\int_{T^d} \boldsymbol{A}(\boldsymbol{k}) d^d k, \tag{8}$$

with $\boldsymbol{r}$ the position operator; the last equality utilizes a known relation between polarization and an integral of the Berry connection $\boldsymbol{A}(\boldsymbol{k})$ [1,77,78]. In this interpretation, a Wannier function centered at $\bar{\boldsymbol{r}}+\boldsymbol{R}$ forms a representation of the site stabilizer $G_{\bar{\boldsymbol{r}}+\boldsymbol{R}}$.

The following lemma is useful to prove our theorem: A sufficient condition for band representability is that a general representation satisfies

$$\forall\, g=(p|\boldsymbol{S}) \in G, \quad \rho_g(\boldsymbol{k}) = \rho_{(p|\boldsymbol{0})}(\boldsymbol{0}) e^{-is_p \check{p}\boldsymbol{k}\cdot\boldsymbol{\Delta}_g}; \tag{9}$$

$$\boldsymbol{\Delta}_g := g\circ\boldsymbol{\varpi} - \boldsymbol{\varpi} \in BL, \tag{10}$$

with g independent $\boldsymbol{\varpi} \in \mathbb{R}^d$. Equations (9) and (10) shall be referred to as the canonical form of a BR [51]. Especially, $\rho_g(\boldsymbol{k})$ depends on $\boldsymbol{S}$ only through Δ_g.

Proof of lemma. Equation (10) is the defining property for a unit-multiplicity Wyckoff position $\boldsymbol{\varpi}$. Any element in $G_{\boldsymbol{\varpi}}$ has the form $p_{\boldsymbol{\varpi}} := (p|-\boldsymbol{\Delta}_{(p|\boldsymbol{0})})$ with $p \in \mathcal{P}$; this reflects an isomorphism with $\mathcal{P}$. Combining Eqs. (9) and (10) with Eq. (7), we derive a unitarily equivalent representation of G on Wannier functions:

$$\forall\, g=(p|\boldsymbol{S}) \in G, \quad \hat{g}\,|w_{\boldsymbol{R}}\rangle = \rho_{(p|\boldsymbol{0})}(\boldsymbol{0})\,|w_{\check{p}\boldsymbol{R}+\boldsymbol{\Delta}_g}\rangle\,. \tag{11}$$

To interpret Eq. (11), $\hat{g}$ has a twofold effect (i) of translating the Wannier center $\boldsymbol{R}+\boldsymbol{\varpi}$ to $g\circ(\boldsymbol{R}+\boldsymbol{\varpi}) = \check{p}\boldsymbol{R}+\boldsymbol{\Delta}_g+\boldsymbol{\varpi}$, and, additionally, (ii) $\hat{g}$ may transform the Wannier function around its own center, thus inducing the phase factor $\rho_{(p|\boldsymbol{0})}(\boldsymbol{0})$. Let us demonstrate that Eq. (11) describes a BR of G. Restricting Eq. (11) to $\boldsymbol{R}=\boldsymbol{0}$ and $p_{\boldsymbol{\varpi}} \in G_{\boldsymbol{\varpi}}$, we derive that $\hat{p}_{\boldsymbol{\varpi}}\,|w_{\boldsymbol{0}}\rangle = \rho_{(p|\boldsymbol{0})}(\boldsymbol{0})\,|w_{\boldsymbol{0}}\rangle$, i.e., $\rho_{(p|\boldsymbol{0})}(\boldsymbol{0})$ is a representation of $G_{\boldsymbol{\varpi}}$ that is restricted from G. One may further verify that $|w_{\boldsymbol{R}}\rangle = \widehat{(E|\boldsymbol{R})}\,|w_{\boldsymbol{0}}\rangle$ [cf. Eq. (7)] forms a representation of

$$G_{\boldsymbol{\varpi}+\boldsymbol{R}} = (E|\boldsymbol{R})\, G_{\boldsymbol{\varpi}}\, (E|\boldsymbol{R})^{-1} \tag{12}$$

for any $\boldsymbol{R} \in BL$, which proves the lemma. ■

It is instructive to demonstrate that the simple band represented by Eqs. (9) and (10) satisfies the conventional [52–54] definition of a BR: as a representation of G that is induced from a representation of a site stabilizer $G_{\boldsymbol{\varpi}}$ on a Wannier function, for some Wyckoff position $\boldsymbol{\varpi}$. Indeed, were we to carry out this induction, we would expand the representation space of $w_{\boldsymbol{0}}$ to include all BL translates of $w_{\boldsymbol{0}}$;[13] these Wannier functions transform as

$$\forall\,(p|\boldsymbol{S}) \in G, \quad \widehat{(p|\boldsymbol{S})}\,|w_{\boldsymbol{R}}\rangle = (E|\check{p}\widehat{\boldsymbol{R}+\boldsymbol{\Delta}}_{(p|\boldsymbol{S})})\hat{p}_{\boldsymbol{\varpi}}\,|w_{\boldsymbol{0}}\rangle\,, \tag{13}$$

from which we recover Eq. (11). This proves that Eq. (11) is a BR as conventionally defined.

V. BAND REPRESENTATIONS ARE TRIVIAL

To recapitulate, a simple BR is a Wannier representation of G, such that each Wannier function represents its site stabilizer. By Fourier transformation [the inverse of Eq. (7)], we obtain a Bloch function that is analytic and periodic [13]. More generally, an N-band BR ($N \geqslant 1$) is analytically trivial, i.e., there exist N Bloch functions which are periodic and analytic, and span the N-band BR at each $\boldsymbol{k}$. Being analytically trivial is generally a stronger condition than being topologically trivial.

VI. A SIMPLE TOPOLOGICALLY TRIVIAL BAND IS A BAND REPRESENTATION

For a simple, topologically trivial band, we have argued that $\psi_{\boldsymbol{k}}$ can be made analytic and periodic; henceforth, these properties are assumed for $\psi_{\boldsymbol{k}}$; it follows from Eq. (2) that both properties are likewise satisfied by $\rho_g(\boldsymbol{k})$. Under this assumption, there remains a freedom to perform gauge transformations [cf. Eq. (6)] with $e^{i\phi(\boldsymbol{k})}$ that is analytic and periodic. Exploiting this freedom, we would show $\rho_g(\boldsymbol{k})$ may be simplified to the canonical form [cf. Eqs. (9) and (10)] for all $g \in G$; according to the lemma in Sec. IV D, this would prove the desired result.

It is not difficult to see that the canonical form applies to the translational subgroup of G: $\rho_{(E|\boldsymbol{R})}(\boldsymbol{k}) = e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}$, as derived in Eqs. (2) and (3). Owing to the simple factorization of ρ_g [cf. Eq. (3)] for symmorphic space groups, what remains is to prove the canonical form for the point-preserving elements of G: $\{(p|\boldsymbol{0})|p \in \mathcal{P}\}$. To simplify notation in the rest of this

[13]Generally, one constructs Wannier functions for all Wyckoff positions in the orbit $G\circ\boldsymbol{\varpi}$; for unit-multiplicity Wyckoff positions, these Wannier functions are just the BL translates of the single Wannier function.

section, we shorten $(p|\mathbf{0})$ to p, e.g., $\rho_{(p|\mathbf{0})} \equiv \rho_p$. We split the proof into three steps, which are to be proven for all $p \in \mathcal{P}$.

(1) A general form for $\rho_p(\boldsymbol{k})$ is

$$\rho_p(\boldsymbol{k}) = e^{-is_p \check{p}\boldsymbol{k}\cdot\boldsymbol{\Delta}_p + i\alpha_p(\boldsymbol{k})}, \quad \text{with } \boldsymbol{\Delta}_p \in BL \tag{14}$$

and $\alpha_p(\boldsymbol{k})$ a real, analytic, periodic function.

(2) There exists $\boldsymbol{\varpi}$ such that $\boldsymbol{\Delta}_p \in BL$ in Eq. (14) satisfies Eq. (10).

(3) By applying a further gauge transformation, the periodic component of the phase of ρ_p [cf. Eq. (14)] may be made independent of $\boldsymbol{k}$: $\alpha_p(\boldsymbol{k}) \to \alpha_p(\mathbf{0})$.

Items 1–3 then imply Eqs. (9) and (10) with the identification $e^{i\alpha_p(\mathbf{0})} = \rho_p(\mathbf{0})$ for all $p \in \mathcal{P}$.

A. Proof of 1

$\rho_p(\boldsymbol{k})$ is a map from the d-torus to $U(1)$, and the homotopy classes of such maps are classified by d integers;[14] these integers may be identified as winding numbers (denoted $n_1, \ldots, n_d \in \mathbb{Z}$) of the $U(1)$ phase over d independent primitive vectors $(\boldsymbol{G}_1, \ldots, \boldsymbol{G}_d) \subset RL$. Equivalently stated, if we define $\theta_p(\boldsymbol{k})$ as the phase of $\rho_p(\boldsymbol{k})$ such that $\theta_p(\boldsymbol{k})$ is analytic throughout $\mathbb{R}^d$, then $\theta_p(\boldsymbol{k}+\boldsymbol{G}_j) = \theta_p(\boldsymbol{k}) + 2\pi n_j$. Without loss of generality, we may decompose θ_p into periodic (α_p) and nonperiodic components as

$$\theta_p(\boldsymbol{k}) = \alpha_p(\boldsymbol{k}) + \boldsymbol{k}\cdot\sum_{i=1}^{d} n_i \boldsymbol{S}_i; \quad \boldsymbol{S}_i \cdot \boldsymbol{G}_j = 2\pi\delta_{ij}, \tag{15}$$

where $\boldsymbol{S}_i \in BL$ are primitive Bravais lattice vectors dual to $\boldsymbol{G}_j$. Since $\sum_i n_i \boldsymbol{S}_i \in BL$ and the Bravais lattice has the symmetry of the point group $\mathcal{P}$, there is no loss in generality in expressing $\sum_i n_i \boldsymbol{S}_i = -s_p \check{p}^{-1} \boldsymbol{\Delta}_p$ with $\boldsymbol{\Delta}_p \in BL$ and $p \in \mathcal{P}$. This completes the proof of 1. ■

B. Proof of 2

Equation (5) constrains the phases of $\rho_p(\boldsymbol{k})$ as

$$s_q \alpha_p(\boldsymbol{k}) + \alpha_q(s_p \check{p}\boldsymbol{k}) - \alpha_{qp}(\boldsymbol{k}) - 2\pi n(q,p) \tag{16}$$

$$= s_{pq}(\check{p}\boldsymbol{k}\cdot\boldsymbol{\Delta}_p + \check{q}\check{p}\boldsymbol{k}\cdot\boldsymbol{\Delta}_q - \check{q}\check{p}\boldsymbol{k}\cdot\boldsymbol{\Delta}_{qp}) \tag{17}$$

for all $p, q \in \mathcal{P}$; $n(q,p) \in \mathbb{Z}$ is introduced to account for the 2π ambiguity of the phase. That $n(q,p)$ is independent of $\boldsymbol{k}$ follows from the analyticity of $\alpha_p(\boldsymbol{k})$ and the integer valuedness of $n(q,p)$.

Let us demonstrate that the left- [Eq. (16)] and right-hand sides [Eq. (17)] of the above equality vanish separately. Since $\alpha_p(\boldsymbol{k})$ is analytic, we may apply the gradient $\boldsymbol{\nabla}_{\boldsymbol{k}}$ to Eqs. (16) and (17):

$$s_q \boldsymbol{\nabla}_{\boldsymbol{k}} \alpha_p(\boldsymbol{k}) + s_p \check{p}^{-1} \boldsymbol{\nabla}_{s_p\check{p}\boldsymbol{k}} \alpha_q(s_p\check{p}\boldsymbol{k}) - \boldsymbol{\nabla}_{\boldsymbol{k}}\alpha_{qp}(\boldsymbol{k}) \tag{18}$$

$$= s_{qp}\check{p}^{-1}(\boldsymbol{\Delta}_p + \check{q}^{-1}\boldsymbol{\Delta}_q - \check{q}^{-1}\boldsymbol{\Delta}_{qp}). \tag{19}$$

The periodicity of α_p and all terms in Eqs. (18) and (19) allows for a Fourier analysis; this demonstrates that $\boldsymbol{\nabla}_{\boldsymbol{k}}\alpha_p(\boldsymbol{k})$ does not contain a constant-in-$\boldsymbol{k}$ term, hence, the bracketed terms in Eq. (19) vanish by linear independence. Summing these bracketed terms over all $q \in \mathcal{P}$ and dividing by the order $(|\mathcal{P}|)$ of $\mathcal{P}$, we derive Eq. (10) with

$$\boldsymbol{\varpi} = \frac{1}{|\mathcal{P}|}\sum_{q\in\mathcal{P}} \check{q}^{-1}\boldsymbol{\Delta}_q. \tag{20}$$

■

C. Proof of 3

Having determined that Eq. (16) vanishes for all $p, q \in \mathcal{P}$, we multiply it by s_q, sum over all $q \in \mathcal{P}$ and divide by $|\mathcal{P}|$ to obtain

$$\alpha_p(\boldsymbol{k}) = s_p\Phi(\boldsymbol{k}) - \Phi(s_p\check{p}\boldsymbol{k}) + \frac{2\pi}{|\mathcal{P}|}\sum_{q\in\mathcal{P}} s_q n(q,p), \tag{21}$$

where $\Phi(\boldsymbol{k}) := \sum_{q\in\mathcal{P}} s_q \alpha_q(\boldsymbol{k})/|\mathcal{P}|$. Since $\Phi(\boldsymbol{k})$ is independent of p, the $\boldsymbol{k}$-dependent terms on the right-hand side of Eq. (21) can be removed by a gauge transformation [Eq. (6)]; we may view this as a transformation between two homotopically equivalent representations.[15] This completes the proof of the theorem. We provide a group-cohomological perspective of $n(q,p)$ as a two-cocyle in Appendix B. ■

VII. GENERALIZATION TO SOLIDS WITH SPIN-ORBIT COUPLING

Our theorem is generalizable to spin-orbit-coupled solids with broken time-reversal symmetry, where the absence of Kramers degeneracy allows for simple bands. The statement of the theorem for spin systems is nearly identical to the spinless case, except G is now identified with a double [79] symmorphic magnetic space group. The proof of the theorem with spin is essentially identical, except $\psi_{\boldsymbol{k}}$ should be replaced by a spinor wave function, and $\mathcal{P} \cong G_{\varpi}$ now includes a nonidentity element [80] corresponding to a 2π rotation.

VIII. APPLICATIONS OF THE THEOREM

Our theorem (including the generalization to half-integer-spin representations in Sec. VII) has two types of applications: the first rules out simple localizable topological bands, which implies a minimal rank for the tight-binding Hamiltonian of localizable topological insulators (Sec. VIII A), and the second guarantees simple Chern insulators (Sec. VIII B). An application to solids with space-time inversion symmetry is highlighted in Sec. VIII C, which illustrates a Stiefel-Whitney obstruction that occurs only for real vector bundles.

[14] This follows because $[T^d, U(1)]$ are in one-to-one correspondence with cohomology classes in $H^1(T^d;\mathbb{Z})$. Applying the universal coefficient theorem, $H^1(T^d;\mathbb{Z}) \cong \mathbb{Z}^d$.

[15] For any two representations $(\rho_p^0(\boldsymbol{k}), \rho_p^1(\boldsymbol{k}))$ of G that are related by a gauge transformation with periodic $\phi(\boldsymbol{k})$, there exists a continuous interpolation $\rho_p^s(\boldsymbol{k})$ $(s \in [0,1])$ that is itself analytic and periodic, and a representation of G throughout the interpolation.

A. A simple band cannot be localizable topological

The following discussion applies in any spatial dimension d, and for G that is symmorphic. A corollary of Theorem 1 states that a simple band cannot be localizable topological, i.e., a localizable topological band minimally has rank two. There are two classes of localizable topological bands distinguished by their stability upon summation[16] with a BR of G: (i) a stable localizable topological band remains localizable topological upon summation (as exemplified by the Kane-Mele phase) [15], while (ii) a fragile localizable topological band becomes band representable upon summation (as exemplified in [55]).

Minimal rank for the tight-binding Hamiltonian of a localizable topological insulator

Restricting our discussion to $d \leqslant 3$, we deduce that the minimal rank of a tight-binding Hamiltonian for a fragile localizable topological insulator is three, and that for a stable localizable topological insulator is four. By "rank" of a tight-binding Hamiltonian, we mean the dimension of the tight-binding Hilbert space as restricted to a wave vector, or to one real-space, primitive unit cell.

Indeed, any G-symmetric tight-binding Hilbert space is a BR of G [7]; this BR must be split to attain a localizable topological band (fragile or topological). Minimally, the tight-binding BR splits into two band subspaces, which we may denote as filled and empty. For a localizable topological filled band, it must be that the empty band is also localizable (i.e., $c_1 = 0$); this follows because the tight-binding BR must be localizable, and the first Chern numbers are stable invariants [81]. If the filled band is stable localizable topological, then so must the empty band (by the definitions of fragile and stable given above), and therefore the combined minimal rank is four. This minimal rank is saturated by the Kane-Mele model [15] of the $\mathbb{Z}_2$ topological insulator, as well as models [43,44] of $\mathbb{Z}_2$ magnetic topological insulators protected by glide symmetry. On the other hand, if the filled band is fragile localizable topological, the empty band may be band representable[17] and its rank is not constrained by our theorem; then, the combined minimal rank is three. This minimal rank is saturated by a kagome model that is detailed below (cf. Sec. VIII B 2).

These rank constraints on the tight-binding Hamiltonian are supported empirically by all localizable, symmorphic topological insulators that we know [[5,6,15–20,23,28–31],[35,38–46,48,60]], including the reflection-symmetric, localizable topological insulators (in Wigner-Dyson symmetry class A and AII) that have been constructed by the minimal-Dirac-Hamiltonian approach [47]. To clarify a difference in methodology, there does not exist (to our knowledge) a rigorous proof that equates the minimal rank of a Dirac Hamiltonian (linear-in-$\boldsymbol{k}$ Hamiltonian with mass terms) with the minimal rank of tight-binding Hamiltonians (having arbitrary dispersion and being defined over the Brillouin torus); in fact, it is known that the former can be larger than the latter, in Altland-Zirnbauer class CI.[18]

We hope our rank constraint will guide future work in constructing tight-binding models of localizable topological insulators. Often a localizable topological insulator is posited to exist by methods such as K-theory [46,59,60], symmetry-based indicator [56], or topological invariants [40,41,82,83], but a tight-binding model for this insulator may not yet be known. The first step in constructing a tight-binding model is to decide the rank of the tight-binding basis functions.

B. Program for high-throughput search of topological materials

In combination with the theory of elementary band representations (EBRs) [51,52,54], our theorem guides the design and identification of Chern and fragile localizable topological insulators. EBRs are the basic building blocks of space-group representations, and serve a role analogous to irreducible representations of finite groups [84]. An EBR is defined as a BR of G which cannot be split into multiple fewer-band subspaces that are all BRs of G; if an EBR of G were splittable, then at least one of the fewer-band subspaces cannot be a BR of G [5–7,55]. Most EBRs satisfy two properties: (i) its Wyckoff position $\boldsymbol{\varpi}$ is maximal, and (ii) the representation of $G_{\boldsymbol{\varpi}}$ is irreducible [5,6,54]; the exceptions to (i) and (ii) are tabulated in the given references.

Whether an EBR is splittable is determined by compatibility relations in combining symmetry representations of little groups over the Brillouin torus [5]; these combinations are tabulated in the Bilbao Crystallographic Server [85] for space groups with and without time-reversal symmetry and $d = 3$. In more detail, under the link "BANDREP," all splittable EBRs of a specified space group are labeled as decomposable; under the link decomposable, all possible connected subspaces (labeled "branch 1," "branch 2," ...) of a splittable EBR are specified by their irreducible representations of little groups at high-symmetry quasimomenta. By a "connected" $N \geqslant 1$ band, we mean that symmetry-enforced band touchings prevent the band from being separated energetically into two or more components; by definition, a simple band is always connected. In symmorphic space groups, a connected subspace may be identified as simple if the representations of all little groups are one dimensional. If one or more of these connected subspaces are simple, our theorem becomes useful in identifying Chern insulators (as discussed in Sec. VIII B 1) and fragile localizable topological insulators (Sec. VIII B 2).

1. Modeling and identifying Chern insulators

If an EBR were splittable into a simple band which is band unrepresentable, then our theorem guarantees that it has a nonzero first Chern class (in short, it is a Chern band). For lower-symmetry space groups, it is not uncommon to find rank-s EBRs that split into $s \geqslant 1$ simple bands; we shall refer

[16]Precisely, we mean a Whitney sum of two vector bundles, where at each $\boldsymbol{k}$ the two vector spaces are directly summed.

[17]In principle, it is possible that both empty and filled bands are fragile localizable topological, in which case the combined rank is minimally four by our theorem.

[18]For 3D class-CI superconductors, the minimal dimension of the Dirac Hamiltonian is eight (see Sec. VI B of [82]), yet Schnyder *et al.* have produced a four-band tight-binding BdG model [112].

to these as "candidate" EBRs. Due to the net topological triviality of all s bands, it follows that at least two of them must be Chern bands. Thus, if $s = 2$, and if the Fermi level separates the two simple bands, a Chern insulator is guaranteed. We have exemplified such EBRs on a two-dimensional (2D) checkerboard lattice ($s = 2$, wallpaper group $P4$), and a 2D honeycomb lattice ($s = 2$, $P6$) in [7].

For $s \geqslant 3$ simple bands, further work is required to determine which of the s simple bands are Chern bands, e.g., by a symmetry representation [24,35,86–89] or a Zak-phase analysis [7]. For illustration, we consider a three-band EBR comprising s orbitals on a kagome lattice (wallpaper group $P6$). In a tight-binding model with (only) imaginary nearest-neighbor hoppings, the EBR splits into three components with first Chern numbers: $C_1 = 0, +1, -1$, respectively [7]; a Chern insulator is attained if the Fermi level separates two subspaces with nontrivial Chern numbers.

For any candidate EBR of a space group G, it is straightforward to design a tight-binding model of the Chern insulator; the tight-binding basis vectors would correspond directly to the Wannier functions that span this EBR [7]. By varying the G-symmetric tight-binding matrix elements, we may explore all possible splittings of this EBR, one of which would give Chern bands.

Finally, to find a naturally occurring Chern insulator from first principles, we propose to search for G-symmetric materials with our candidate EBR in the vicinity of the Fermi level. Let us outline our proposed method: (a) from Bilbao, identify all candidate EBRs for a space group G and record their irreducible representations at high-symmetry quasimomenta (in short, we will refer to these representations as symmetry indicators). (b) Identify several candidate materials with the same space group. (c) For a band subspace near the Fermi level of a candidate material, identify and compare their symmetry indicators to that of the candidate EBRs. Band subspaces whose indicators match with (at least)[19] one candidate EBR shall be referred to as candidate bands. (d) Symmetry indicators alone do not guarantee that the candidate band is a candidate EBR; in principle, it is possible that the same symmetry indicators are shared by two distinct EBRs [54], or even by an EBR and a localizable topological band [5,55]. One way to guarantee that a candidate band is a candidate EBR is as follows: construct the locally symmetric Wannier functions that one expects for the candidate EBR. Assuming this is done, then one may directly apply the discussion in the first two paragraphs (of this section) to identify Chern bands.[20] (e) The task of constructing locally symmetric Wannier functions may be numerically intensive, and to our knowledge a standard software does not yet exist in the first-principles community. Pragmatically, one may avoid this and directly compute the Chern numbers of the simple bands (which comprise the candidate band). For such a computation, there already exist standard software [90] which utilize Wilson-loop techniques.

2. *Identifying fragile localizable topological insulators*

Suppose a rank-s EBR splits into two orthogonal subspaces (S_1, S_2), each of which is not necessarily connected. Then, if S_1 is band representable, S_2 must be fragile localizable topological. If S_1 comprises of simple band(s) with vanishing first Chern number(s), then our theorem guarantees that S_1 is band representable. An illustration is provided by splitting the same kagome EBR just described in Sec. VIII B 1: If S_1 is the simple band with $C_1 = 0$, then S_2 is composed of two simple bands with $C_1 = +1, -1$, and must therefore be fragile localizable topological. One manifestation of this fragile topology is a nontrivial winding of the eigenvalues of the holonomy matrix (i.e., Wilson loop).[21]

Our theorem has greatest utility in magnetic space groups which guarantee the triviality of the first Chern class [e.g., time-reversal symmetry, or $(d-1)$ orthogonal mirror symmetries in a d-dimensional cubic lattice]. For such groups, S_1 is guaranteed to be band representable by our theorem. As an application, let us search in Bilbao for the following EBR of space group 183 with time-reversal symmetry: this EBR is labeled by the Wyckoff position $\boldsymbol{\varpi} = 3c$, and a trivial onsite symmetry representation A_1 of the onsite stabilizer $G_{\boldsymbol{\varpi}} = C_{2v}$. This rank-three EBR is splittable into a simple band (branch 1) and a pair of bands (branch 2); the latter must be fragile localizable topological.

C. Application to bands with space-time inversion symmetry

We remark on a class of bands that arise in solids with negligible spin-orbit coupling, and the symmetry of space-time inversion: $(\boldsymbol{r}, t) \to (-\boldsymbol{r}, -t)$. This symmetry ensures that $h(\boldsymbol{k})$, the tight-binding Hamiltonian, can be made real at each $\boldsymbol{k}$, as explained in Appendix C. The real eigenvectors of $h(\boldsymbol{k})$ (corresponding to the filled bands) define a real vector bundle which is guaranteed to have vanishing first Chern class by the space-time inversion symmetry. Since a real vector bundle (or real band) can be embedded in a complex one (in analogy with how real numbers can be embedded in complex numbers) [57], our theorem also applies to real bands of symmorphic magnetic space group G; in fact, the theorem directly implies that any real simple band with G symmetry is necessarily a BR of G.

Despite being trivial when viewed as a complex unit-rank (i.e., line) bundle, a real simple band may nevertheless be nontrivial in the category of real line bundles. Triviality in the category of real line bundles is equivalent [62] to the vanishing of the first Stiefel-Whitney characteristic class, or equivalently to the existence of a real section [a real eigenvector $|u_{\boldsymbol{k}}\rangle$ of $h(\boldsymbol{k})$ that is continuous, periodic, and nonvanishing over T^d]. The latter implies that the Berry connection $i\,\langle u_{\boldsymbol{k}}|\nabla_{\boldsymbol{k}} u_{\boldsymbol{k}}\rangle$ (being necessarily real) must vanish at all $\boldsymbol{k}$, and hence the Berry-Zak phase vanishes for the holonomy over all

[19] In principle, it is possible that two EBRs share the same symmetry indicators [54].

[20] If one finds that a candidate band is not band representable, then it must either be a nonsimple Chern band or a localizable topological band.

[21] It is characterized by a unit relative winding number, a topological invariant first discovered in [41]. This invariant has also been used to characterize other fragile phases [49].

noncontractible Brillouin-zone loops. Utilizing the geometric theory of polarization [77], we deduce that the corresponding Wannier center lies at the spatial origin, modulo translations by a Bravais-lattice vector.

An obstructed simple real band is exemplified by either of the two energy bands of the Hamiltonian $h(k) = \cos(k)\sigma_3 + \sin(k)\sigma_1$, which is real at all $k \in T^1$ (σ_1, σ_3 are Pauli matrices). A real eigenvector of $h(k)$ that is continuous at each k must satisfy antiperiodic boundary conditions over T^1, i.e., the Zak phase is π. This relation between the first Stiefel-Whitney class and the Zak phase was independently discovered in [91]. An analytic and periodic eigenvector can be attained by multiplying the real eigenfunctions of $h(k)$ by a complex phase factor $e^{ik/2}$ [cf. Eq. (6)]; the corresponding Wannier function is necessarily displaced by half a lattice period (modulo lattice translations) from the origin.

We remark that a simple BR of G can also be nontrivial in the category of G-equivariant [59] line bundles, with G a space group. In fact, $h(k)$ above also has the reflection symmetry $\sigma_3 h(k)\sigma_3 = h(-k)$, and the filled band of $h(k)$ exemplifies a nontrivial reflection-equivariant line bundle.

IX. DISCUSSION AND OUTLOOK

The question of the minimal rank of a band subspace is increasingly enriched by the interplay between band topology and crystallographic symmetry [24,76,92,93]. A space-group-symmetric band subspace may be topologically trivial, yet its rank exceeds unity if there exists symmetry-enforced band-touching points in T^d. These touchings are associated to higher-than-one-dimensional irreducible representations of the little group at high symmetry $\boldsymbol{k} \in T^d$ [94,95] or to the nontrivial monodromy of nonsymmorphic symmetry representations [7,76,92,93,96]. This local-in-$\boldsymbol{k}$ perspective of symmetry representations contrasts with a global perspective that is required to understand topological band insulators. A case in point are insulators with a nontrivial second (or higher) Chern class; their rank must exceed unity [62], independent of the presence of crystallographic symmetry.

In this work, we present a rank constraint that relies saliently on both band topology and crystallographic point-group symmetry: the rank of a localizable topological band must exceed unity. To recapitulate, we have defined a localizable topological band as having an obstruction to locally symmetric Wannier functions, i.e., it is a localizable band that is not a band representation (BR). This local symmetry condition has been defined in our Introduction, and a more elaborate definition may be found in Appendix A. Our rank constraint is fundamentally different from those imposed by symmetry-enforced touching points in $\boldsymbol{k}$ space, e.g., a fragile localizable topological band may be a sum of simple bands with no such touching points, as exemplified by the kagome model in Sec. VIII B 2.

An alternative restatement of this rank constraint is that the phase diagram of unit-rank band subspaces (simple bands) is comparatively uncomplicated, as illustrated in Figs. 1(a) and 1(b): either a simple band is unlocalizable (with a nontrivial first Chern class) or otherwise it is a BR. Our rank constraint is the corollary of a theorem that states the following: for simple bands, being a band representation is equivalent to being topologically trivial in the category of complex vector bundles. It should be emphasized that our theorem applies generally to space-group-symmetric band systems, independent of the statistics of particles that fill the band. In particular, the applications extend to bosonic band systems such as photonic crystals [97,98], phonon bands [99,100], and linear circuit lattices [67–69].

Finally, we remark on our definition of a BR as unitarily equivalent to locally symmetric Wannier functions. *A priori*, this definition is not obviously equivalent to the conventional definition [51–54] of BRs as induced representations of space groups; this equivalence is proven in Appendix A. Arguably, our unconventional definition more directly and intuitively pinpoints the difference between BRs and localizable topological bands.

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APPENDIX A: EQUIVALENCE OF DEFINITIONS OF BAND REPRESENTATION

Two equivalent definitions for band representations (BRs) of space groups exist: one from the perspective of inducing a representation of site stabilizer, and another from the dual perspective of restricting a localizable representation of a space group to a site stabilizer. In this appendix, we prove their equivalence.

1. General definition of localizable representations

Let us first define a rank-($N \geqslant 1$) localizable representation of a magnetic space group G (symmorphic or nonsymmorphic).

Definition 1. A *localizable representation of* G is an infinite-dimensional linear representation of G on Wannier functions $\{|w^{\alpha_n}_{n,\boldsymbol{R}}\rangle\}_{\alpha_n,n,\boldsymbol{R}}$ where $\boldsymbol{R} \in BL$, n labels distinct Wannier centers $\boldsymbol{\varpi}_n$ in one unit cell, and α_n distinguishes Wannier functions centered on the same coordinate $\boldsymbol{\varpi}_n$.

Here and throughout this paper, Wannier functions are defined to be exponentially localized Fourier transforms of Bloch functions:

$$w^{\alpha_n}_{n,\boldsymbol{R}}(\boldsymbol{r}) = \sum_{m,\beta_m} \int_{T^d} \frac{e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}}{\sqrt{|T^d|}} [U(\boldsymbol{k})]^{\beta_m,\alpha_n}_{m,n} \psi^{\beta_m}_{m,\boldsymbol{k}}(\boldsymbol{r}) d\boldsymbol{k}. \quad \text{(A1)}$$

The Bloch functions $\{\psi^{\beta_m}_{m,\boldsymbol{k}}\}_{m,\beta_m}$ are assumed to be analytic and periodic, and they orthonormally span the N-dimensional

vector space at each $\boldsymbol{k}$. As explained in the main text, such Bloch functions exist if and only if the $(N \geqslant 1)$-band subspace is topologically trivial as a complex vector bundle [101–103]. $U(\boldsymbol{k})$, when viewed as a matrix with row index (m, β_m) and column index (n, α_n), is unitary, periodic, and analytic. The presence of this matrix in Eq. (A1) reflects a choice of basis (or "gauge freedom") for the Wannier functions [104]. It follows from Eq. (A1) all Wannier functions labeled by the same n and α_n are related by Bravais-lattice translations:

$$\left|w^{\alpha_n}_{n,\boldsymbol{R}}\right\rangle = \widehat{(E|\boldsymbol{R})}\left|w^{\alpha_n}_{n,\boldsymbol{0}}\right\rangle. \tag{A2}$$

This is a convenient choice of basis that exploits the discrete translational symmetry.

In Definition 1, we have organized Wannier functions according to their Wannier centers, which are defined as expectation values of the position operator [cf. Eq. (8) for a simple band]:

$$\boldsymbol{\varpi}_n + \boldsymbol{R} = \left\langle w^{\alpha_n}_{n,\boldsymbol{R}}\right| \boldsymbol{r} \left|w^{\alpha_n}_{n,\boldsymbol{R}}\right\rangle. \tag{A3}$$

The number of Wannier functions centered on $\boldsymbol{\varpi}_n$ might vary with n; the total number of Wannier functions centered within one unit cell is N.

It is useful to define a special type of localizable representation:

Definition 2. A *localizable representation of G with a single Wyckoff position $\boldsymbol{\varpi}$* is a localizable representation of G where all Wannier centers are related to $\boldsymbol{\varpi}$ by symmetry.

We may take $\boldsymbol{\varpi} := \boldsymbol{\varpi}_1$, and define the site stabilizer $G_{\boldsymbol{\varpi}}$ is the subgroup of G that preserves $\boldsymbol{\varpi}$. Definition 2 implies, for each $n = 1, \ldots, M$, there exists a representative element $g_n \in \mathcal{P}/G_{\boldsymbol{\varpi}}$ such that $g_n \circ \boldsymbol{\varpi} = \boldsymbol{\varpi}_n$, with g_1 being the identity element. $M = |\mathcal{P}|/|G_{\boldsymbol{\varpi}}|$ is defined as the multiplicity of the Wyckoff position $\boldsymbol{\varpi}$. It follows from Eq. (A3) that $\hat{g}_n \left|w^{\alpha_1}_{1,\boldsymbol{0}}\right\rangle$ is centered at $\boldsymbol{\varpi}_n$, hence the space orthonormally spanned by $\{\hat{g}_n \left|w^{\alpha_1}_{1,\boldsymbol{0}}\right\rangle\}_{\alpha_1}$ is a subspace of the space orthonormally spanned by $\{\left|w^{\alpha_n}_{n,\boldsymbol{0}}\right\rangle\}_{\alpha_n}$; conversely, we may demonstrate that the space spanned by $\{\hat{g}_n^{-1} \left|w^{\alpha_n}_{n,\boldsymbol{0}}\right\rangle\}_{\alpha_n}$ is a subspace of the space spanned by $\{\left|w^{\alpha_1}_{1,\boldsymbol{0}}\right\rangle\}_{\alpha_1}$. Clearly then $\hat{g}_n$ is an isomorphism between two vector spaces, and we may as well define

$$\left|w^{\alpha}_{n,0}\right\rangle = \hat{g}_n \left|w^{\alpha}_{1,0}\right\rangle, \tag{A4}$$

for all n, α; presently, we may drop the subscript of α_n.

We remark that any localizable representation of G is a direct sum of single-Wyckoff localizable representations (possibly with distinct Wyckoff positions).

2. Conventional definition of band representations

A BR is a special type of localizable representation [51,52].

Definition 3: A *band representation of G with Wyckoff position $\boldsymbol{\varpi}$* is the induced representation of $G_{\boldsymbol{\varpi}} \subset G$. A direct sum of band representations (possibly with distinct Wyckoff positions) is also referred to as a band representation.

In more detail, inducing a finite-dimensional representation V of $G_{\boldsymbol{\varpi}}$ on Wannier functions $\{\left|w^{\alpha}_{1,0}\right\rangle\}_{\alpha=1}^{\dim V}$ gives an infinite-dimensional representation of G on Wannier functions $\{\left|w^{\alpha}_{n,\boldsymbol{R}}\right\rangle\}_{\alpha,n,\boldsymbol{R}}$ where $\boldsymbol{R} \in BL$, $\alpha = 1, \ldots, \dim V$; $n = 1, \ldots, M$ with M the multiplicity as defined above. This induced representation is a localizable representation of G with a single Wyckoff position $\boldsymbol{\varpi}$, for which Wannier functions can be chosen to satisfy Eqs. (A2)–(A4). The induced representation on such Wannier functions is, for all $g = (p|\boldsymbol{t}) \in G$ [7,53],

$$\hat{g}\left|w^{\alpha}_{n,\boldsymbol{R}}\right\rangle = \sum_{\beta=1}^{\dim V} \left[V\left(p^{-1}_{n'} p p_n\right)\right]_{\beta\alpha} \left|w^{\beta}_{n',\check{p}\boldsymbol{R}+\Delta_{g,n',n}}\right\rangle,$$
$$\Delta_{g,n',n} = g \circ \boldsymbol{\varpi}_n - \boldsymbol{\varpi}_{n'} \in BL, \tag{A5}$$

where the action of g on a vector $\boldsymbol{r}$ is $g \circ \boldsymbol{r} = \check{p}\boldsymbol{r} + \boldsymbol{t}$; if g is a nonsymmorphic element, then $\boldsymbol{t}$ is not a Bravais-lattice vector.

To motivate the form of Eq. (A5), the action of $\hat{g}$ on Wannier functions may be separated into two effects: (i) a translation of the Wannier center from

$$\boldsymbol{\varpi}_n + \boldsymbol{R} \to g \circ (\boldsymbol{\varpi}_n + \boldsymbol{R}) = \boldsymbol{\varpi}_{n'} + \check{p}\boldsymbol{R} + \Delta_{g,n',n}, \tag{A6}$$

as well as (ii) a local transformation of Wannier functions sharing the same center, as effected by the matrix $V(p^{-1}_{n'} p p_n)$. To motivate the argument of V, observe that $p^{-1}_{n'} p p_n$ is the origin-preserving component of $g^{-1}_{n'}(E|-\Delta_{g,n',n}) g g_n$, which consecutively maps $\boldsymbol{\varpi} \to \boldsymbol{\varpi}_n \to g \circ \boldsymbol{\varpi}_n \to \boldsymbol{\varpi}_{n'} \to \boldsymbol{\varpi}$. This implies that $g^{-1}_{n'}(E|-\Delta_{g,n',n}) g g_n$ is an element in the site stabilizer $G_{\boldsymbol{\varpi}}$, and V a representation of $G_{\boldsymbol{\varpi}}$. Note further that for all $g = (p|\boldsymbol{t}) \in G_{\boldsymbol{\varpi}}$, the set $(p|\boldsymbol{0})$ forms an isomorphic point group related to $G_{\boldsymbol{\varpi}}$ by conjugation, hence, we may as well label $V(g)$ by $V(p)$, as we have done in Eq. (A5).

Corresponding to Eq. (A5) is the following representation of G on $N = M \times \dim V$ Bloch functions [7,53]:

$$[\rho_g(\boldsymbol{k})]^{\beta,\alpha}_{n',n} = e^{-i s_p \check{p}\boldsymbol{k}\cdot\Delta_{g,n',n}} \left[V\left(p^{-1}_{n'} p p_n\right)\right]_{\beta\alpha}; \tag{A7}$$

this may be derived by combining Eqs. (A5) and (A1), with the choice $[U(\boldsymbol{k})]^{\beta,\alpha}_{m,n} = \delta_{m,n}\delta_{\beta,\alpha}$. $\rho_g(\boldsymbol{k})$, when viewed as a matrix with row index (β, n') and column index (α, n), is unitary. Equations (A5) and (A7) are the generalizations of Eqs. (9)–(11) to $M \geqslant 1$ and $\dim V \geqslant 1$.

3. Equivalent definition of band representations

We now provide an equivalent definition of a band representation by restricting representations of space groups to site stabilizers.

Definition 4: A *band representation of G with Wyckoff position $\boldsymbol{\varpi}$* is a localizable representation of G with $\boldsymbol{\varpi}$, such that for all n and all $\boldsymbol{R} \in BL$, $\{\left|w^{\alpha}_{n,\boldsymbol{R}}\right\rangle\}_{\alpha}$ forms a representation of the site stabilizer $G_{\boldsymbol{\varpi}_n+\boldsymbol{R}}$.

Definition 4 means that for all $n = 1, \ldots, M$ (the multiplicity) and all $\boldsymbol{R} \in \mathrm{BL}$, there exists a finite-dimensional unitary representation $X_{n,\boldsymbol{R}}(p)$ of $G_{\boldsymbol{\varpi}_n+\boldsymbol{R}}$, i.e., for all $g = (p|\boldsymbol{S}) \in G_{\boldsymbol{\varpi}_n+\boldsymbol{R}}$:

$$\hat{g}\left|w^{\alpha}_{n,\boldsymbol{R}}\right\rangle = \sum_{\beta=1}^{\dim X_{n,\boldsymbol{R}}} [X_{n,\boldsymbol{R}}(p)]_{\beta,\alpha} \left|w^{\beta}_{n,\boldsymbol{R}}\right\rangle. \tag{A8}$$

In comparison, for any localizable representation of G, the full representation space $\{\left|w^{\alpha}_{n,\boldsymbol{R}}\right\rangle\}_{\alpha,n,\boldsymbol{R}}$ forms a representation of any subgroup of G. Since g_n and $(E|\boldsymbol{R})$ act bijectively on Wannier centers [cf. Eq. (A3)], they also induce an isomorphism of vector spaces spanned by Wannier functions [whose centers are related through Eq. (A3)]; an analogous

demonstration has been provided in Sec. A 1. Consequently, we may as well define Eqs. (A2) and (A4) for all n, α, and $\boldsymbol{R}$, which implies dim $X_{n,\boldsymbol{R}}$ is independent of n and $\boldsymbol{R}$.

We would now prove the equivalence of Definitions 3 and 4. It is sufficient to prove the equivalence for BRs with a single Wyckoff position since BRs characterized by multiple Wyckoff positions are direct sums of single-Wyckoff BRs.

Proof. That Definition 3 implies Definition 4 is straightforward: recalling the definition of the site stabilizer G_{ϖ_n+R} as the subgroup of G which preserves $\boldsymbol{\varpi}_n+\boldsymbol{R}$, we may restrict Eq. (A5) to $g=(p|\boldsymbol{t})\in G_{\varpi_n+R}$ by fixing $n'=n$ and $\check{p}\boldsymbol{R}+\Delta_{g,n',n}=\boldsymbol{R}$. Then, Eq. (A8) follows for $X_{n,\boldsymbol{R}}(p)=V(p_n^{-1}pp_n)$.

Let us now prove the converse: beginning from Definition 4 and Eq. (A8), we would derive Eq. (A5) which gives Definition 3. Utilizing Eq. (A4), we first show that $X_{n,\boldsymbol{R}}(p)$ is independent of $\boldsymbol{R}$: applying that $G_{\boldsymbol{\varpi}_n}$ is conjugate to $G_{\varpi_n+R}=(E|\boldsymbol{R})G_{\varpi_n}(E|\boldsymbol{R})^{-1}$ [cf. Eq. (12)], for any $(p|\boldsymbol{T})\in G_{\varpi_n+R}$ there exists $(p|\boldsymbol{S})\in G_{\varpi_n}$ such that

$$[X_{n,\boldsymbol{R}}(p)]_{\beta,\alpha}=\langle w^{\beta}_{n,\boldsymbol{R}}|\widehat{(p|\boldsymbol{T})}|w^{\alpha}_{n,\boldsymbol{R}}\rangle =\langle w^{\beta}_{n,\boldsymbol{0}}|\widehat{(p|\boldsymbol{S})}|w^{\alpha}_{n,\boldsymbol{0}}\rangle=[X_{n,\boldsymbol{0}}(p)]_{\beta,\alpha}. \tag{A9}$$

Utilizing Eq. (A4), one may similarly show that

$$X_{n,\boldsymbol{0}}(p)=X_{1,\boldsymbol{0}}\big(p_n^{-1}pp_n\big). \tag{A10}$$

Inserting Eqs. (A9) and (A10) into Eq. (A8), we derive that for all $g\in G_{\varpi_n+R}$,

$$\hat{g}\,|w^{\alpha}_{n,\boldsymbol{R}}\rangle=\sum_{\beta=1}^{\dim X_{1,\boldsymbol{0}}}\big[X_{1,\boldsymbol{0}}\big(p_n^{-1}pp_n\big)\big]_{\beta,\alpha}\,|w^{\beta}_{n,\boldsymbol{R}}\rangle. \tag{A11}$$

To complete the proof, we would employ a previous observation that $g_{n'}^{-1}(E|-\Delta_{g,n',n})gg_n\in G_{\varpi}$; this implies that any $g\in G$ can be decomposed into the product $g=(E|\Delta_{g,n',n})g_{n'}hg_n^{-1}$ for some $h\in G_{\varpi}$. Given the representations of h [cf. Eq. (A11)], g_n, $g_{n'}$ [cf. Eq. (A4)], and $(E|\Delta_{g,n',n})$ [cf. Eq. (A2)], we finally derive that Eq. (A8) implies Eq. (A5) with the identification $X_{1,\boldsymbol{0}}=V$. This finishes the proof of the equivalence. ∎

APPENDIX B: COHOMOLOGICAL INTERPRETATION OF $n(q,p)$

In the canonical gauge where α_p is $\boldsymbol{k}$ independent, the left-hand side of Eq. (16) (which vanishes according to Sec. VI B) reduces to

$$2\pi n(q,p)=s_q\alpha_p(\boldsymbol{0})+\alpha_q(\boldsymbol{0})-\alpha_{qp}(\boldsymbol{0}). \tag{B1}$$

The aim of this appendix is to identify $n(q,p)$ as an inhomogeneous 2-cocycle, and the equivalence classes of $n(q,p)$ (specified below) as classifying the 1D linear representations of the point group $\mathcal{P}$.

To begin, let us review a few notions from group cohomology, as particularized to the present context. For a group H, we define the H module as an Abelian group on which H acts compatibly with the multiplication operation. In our context, we consider the $\mathcal{P}$ module $\mathbb{Z}_T$, which equals $\mathbb{Z}$ as a set, and is endowed with an action (denoted $\cdot$) of an element $p\in\mathcal{P}$ on an element $m\in\mathbb{Z}_T$: $p\cdot m=s_pm$ [105,106]. The associativity condition $\alpha_{q(pr)}(\boldsymbol{0})=\alpha_{(qp)r}(\boldsymbol{0})$ implies that $n(q,p)$ is an inhomogeneous 2-cocycle, i.e., a map from from $\mathcal{P}\times\mathcal{P}$ to $\mathbb{Z}_T$ satisfying that

$$0=n(qp,r)+n(q,p)-n(q,pr)-s_qn(p,r);$$

the right-hand side may be identified as an inhomogeneous 3-coboundary. Since α_p is a phase it has a 2π ambiguity, and $n(q,p)$ is only well-defined modulo:

$$\alpha_p(\boldsymbol{0})\to\alpha_p(\boldsymbol{0})+2\pi\mathcal{Q}(p),\quad \mathcal{Q}(p)\in\mathbb{Z},$$
$$n(q,p)\to n(q,p)+s_q\mathcal{Q}(p)+\mathcal{Q}(q)-\mathcal{Q}(qp). \tag{B2}$$

The rightmost three terms may be viewed as an inhomogeneous 2-coboundary. Defining an equivalence for $n(q,p)$ modulo 2-coboundaries, the equivalence classes of such $n(q,p)$ define [105,107] the second group cohomology: $H^2(\mathcal{P},\mathbb{Z}_T)$; this is isomorphic to $H^1(\mathcal{P},U(1)_T)$ [105], where $U(1)_T$ is defined as $U(1)$ that is complex conjugated under the action of time-reversing elements of $\mathcal{P}$. In fact, $H^1(\mathcal{P},U(1)_T)$ is known to classify all the inequivalent 1D linear representations $[e^{i\alpha_p(\boldsymbol{0})}\in U(1)]$ of $\mathcal{P}$ [105].

APPENDIX C: REALITY DUE TO SPACE-TIME INVERSION SYMMETRY

In a space-time inversion symmetric insulator without spin-orbit coupling [i.e., with spin SU(2) symmetry], there exists an antiunitary operator $\tilde{T}$ which is a symmetry of the Schrödinger Hamiltonian H_0 and squares to identity. We may work in a spinor basis $f_s(\boldsymbol{r})$ where $s=\pm1$ corresponds to spin up and down in the z direction; in this basis, $\tilde{T}=e^{i\pi\sigma_y/2}T\mathcal{I}$ is the composition of a π-spin rotation about the y axis (a symmetry of the Hamiltonian), the time-reversal operator $T=e^{-i\pi\sigma_y/2}K$ (with K implementing complex conjugation and $T^2=-1$), and the spatial-inversion operator $\mathcal{I}$ which maps $\boldsymbol{r}\to-\boldsymbol{r}$. In composition, $\tilde{T}=K\mathcal{I}$ preserves the spin component S_z, i.e., $\tilde{T}f_s(\boldsymbol{r})=\bar{f}_s(-\boldsymbol{r})$.

We now study how $\tilde{T}$ is represented on the Fourier transform of an orthonormal tight-binding basis corresponding to Löwdin-orthogonalized orbitals $|\phi_{\alpha,\boldsymbol{R}}\rangle$, where $\alpha=1,\ldots,N$ is orbital index and $\boldsymbol{R}$ a BL, i.e., on

$$|u_{\alpha,\boldsymbol{k}}\rangle_{\text{cell}}=\frac{1}{\sqrt{|T^d|}}\sum_{\boldsymbol{R}}e^{i\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{r})}\,|\phi_{\alpha,\boldsymbol{R}}\rangle_{\text{cell}}\,. \tag{C1}$$

$\langle\,.\,|\,.\,\rangle_{\text{cell}}$ denotes the inner product over one unit cell. The tight-binding Hamiltonian is defined as the matrix elements of the Hamiltonian H_0 in this basis:

$$[h(\boldsymbol{k})]_{\alpha\beta}=\langle u_{\alpha,\boldsymbol{k}}|e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}H_0e^{i\boldsymbol{k}\cdot\boldsymbol{r}}|u_{\beta,\boldsymbol{k}}\rangle_{\text{cell}}. \tag{C2}$$

The unitary component of the representation of $\tilde{T}$ is [36]

$$[\mathcal{B}(\boldsymbol{k})]_{\beta\alpha}=\langle u_{\beta,\boldsymbol{k}}|\tilde{T}|u_{\alpha,\boldsymbol{k}}\rangle_{\text{cell}}=\int_{\text{cell}}\bar{u}_{\beta,\boldsymbol{k}}(\boldsymbol{r})\bar{u}_{\alpha,\boldsymbol{k}}(-\boldsymbol{r})d\boldsymbol{r}; \tag{C3}$$

one may verify that this matrix is unitary

$$\sum_{\gamma=1}^{N}[\mathcal{B}(\boldsymbol{k})]_{\alpha\gamma}[\bar{\mathcal{B}}(\boldsymbol{k})]_{\beta\gamma}=\langle u_{\alpha,\boldsymbol{k}}|u_{\beta,\boldsymbol{k}}\rangle_{\text{cell}}=\delta_{\alpha,\beta}, \tag{C4}$$

and symmetric $[\mathcal{B}(\boldsymbol{k})]_{\beta\alpha}=[\mathcal{B}(\boldsymbol{k})]_{\alpha\beta}$.

We now show that there exists a basis of $|u_{\alpha,\boldsymbol{k}}\rangle$ for which $h(\boldsymbol{k})$ is real and symmetric at each $\boldsymbol{k}$. $[\tilde{T}, H] = 0$ implies that

$$\begin{aligned} h(\boldsymbol{k})_{\beta\alpha} &= \langle u_{\beta,\boldsymbol{k}}|e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} H_0 e^{i\boldsymbol{k}\cdot\boldsymbol{r}}|u_{\alpha,\boldsymbol{k}}\rangle_{\text{cell}} \\ &= \langle u_{\beta,\boldsymbol{k}}|\tilde{T} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} H_0 e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \tilde{T}|u_{\alpha,\boldsymbol{k}}\rangle_{\text{cell}} \\ &= [\mathcal{B}(\boldsymbol{k})]_{\beta\gamma} \bar{h}(\boldsymbol{k})_{\gamma\delta} [\bar{\mathcal{B}}(\boldsymbol{k})]_{\delta\alpha} \\ &= [\mathcal{B}(\boldsymbol{k})\bar{h}(\boldsymbol{k})\bar{\mathcal{B}}(\boldsymbol{k})]_{\beta,\alpha}, \end{aligned} \tag{C5}$$

using the Einstein summation convention. The symmetric matrix $\mathcal{B}(\boldsymbol{k})$ can be diagonalized by an orthogonal matrix $S(\boldsymbol{k})$: $\mathcal{B}(\boldsymbol{k}) = S(\boldsymbol{k})D(\boldsymbol{k})S^T(\boldsymbol{k})$ where ^{T} denotes transposition. D is a diagonal matrix with unimodular diagonal entries, and therefore $D^{-1}(\boldsymbol{k}) = \bar{D}(\boldsymbol{k})$. We now implement the unitary transformation $U(\boldsymbol{k}) = S(\boldsymbol{k})D^{1/2}(\boldsymbol{k})$ [43], such that the transformed Hamiltonian is real at each $\boldsymbol{k}$:

$$\begin{aligned} h' := U^\dagger h U &= D^{-1/2} S^T \left(SDS^T \bar{h} S \bar{D} S^T\right) S D^{1/2} \\ &= D^{1/2} S^T \bar{h} S D^{-1/2} = \bar{h}'. \end{aligned} \tag{C6}$$

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